EPA Comments on Food Web Modeling Report: Evaluating TrophicTrace and the Arnot and Gobas Models for Application to the Portland Harbor Superfund Site (November 2005 Draft)

#### **General Comments:**

It should be noted that the comments provided below are focused on the food web model approach. Detailed comments on the LWG's parameterization of the model require runs of the model, which has not yet been completed by the government team.

Model Objectives: On May 31, 2005, EPA provided to the LWG a list of five food web modeling objectives, as well as nine food web modeling specifications EPA and its partners believes the Portland Harbor food web model must fulfill in order for the model to meet the defined modeling objectives. These modeling objectives and specifications were reiterated to LWG on July 29, 2005. Based on the presentation of LWG's model objectives and specifications in it's November 4, 2005 Draft Food Web Modeling Report, EPA has identified a lack of concordance between the LWG's modeling objectives and specifications and the objectives and specifications as defined by EPA. One notable example is EPA's Objective 4: ability to incorporate temporal variability. Steady state models such as Arnot and Gobas in the form used by LWG cannot explicitly incorporate temporal variation into the model. This means the current modeling efforts will not be able to predict the length of time needed following remediation for fish tissue concentrations to reach acceptable risk levels. Until the differences in the overall modeling objectives and specifications are reconciled, EPA believes it is premature to provide complete comments on the results and conclusions of the draft report, as it is uncertain whether all of EPA's model objectives and specifications can be attained by LWG's modeling approach. EPA is providing comments on those aspects of LWG's modeling approach where a steady state model can meet our modeling objectives and specifications. However, there needs to be agreement between EPA and LWG on modeling objectives and specifications before additional modeling takes place, so that LWG's modeling efforts can continue to advance the RI/FS process.

<u>Model Selection</u>: For modeling objectives and specifications that can be performed with a steady state model of organic compounds, the Arnot and Gobas model is acceptable for use at Portland Harbor. However, it is discouraging that the model performance, in general, did not improve over that described in the LWG's initial FWM report. Focusing on one model should free-up time to improve the efficiency of the sensitivity and uncertainty analysis processes, parameterization, and to begin developing a transport and fate model to accompany the food web model.

<u>Develop Appropriate Scale for Food Web Model</u>: The Food Web Model Report considered two spatial scales – Large Scale (RM 2 – 11) and Small Scale (Swan Island Lagoon). The scale question has significant implications for the human health and ecological risk assessments, the feasibility study and the site cleanup decisions. Future iterations of the food web model should consider breaking the river into a series of segments to facilitate evaluation of the relationship between contaminant sources and tissue concentrations and decision making. Factors that will affect scale include physical features (e.g., hydrodynamics and habitat), exposure considerations

(e.g., receptor home range), contaminant distribution and data availability. Further discussion is required to determine the appropriate scale of the food web model.

Identify Chemicals to be Modeled and how to Address Chemical Mixtures: The current modeling effort is focused on two contaminants – PCB Aroclors (a mixture) and 4,4-DDE. Further discussion is required to determine which chemicals should be modeled in the food web model. Key questions include how to address chemical mixtures, whether to model PAHs, how to model PCB congeners, and what other chemicals to model. Preliminary screening of contaminants detected in fish tissue (e.g., as presented in the PRE and/or the results of human health screening) may facilitate the selection of chemicals to be modeled.

<u>Identify Steps to Improve Model Performance</u>: More extensive analysis is required to understand why the model failed to accurately predict contaminant concentrations in biota. As described in the report, two compounds are selected to test the model. Criteria for selecting these two compounds include a reasonably robust supporting data set and variability for a key parameter (K<sub>ow</sub>) that can be used to help determine if the model(s) can be accurately parameterized. The test runs for the sensitivity and uncertainty analyses provide a substantial amount of information regarding how the models are running, but the report fails to fully discuss the reasons for the results and how those might affect the use of the models. To provide additional clarity, it may be useful to consider, for example, whether one or a few fish species were consistently modeled well. In those instances where this proves to be the case, consideration should be given to uniqueness (e.g., small home range, particular diet, etc.). Similarly, for species where the model does not perform well, what features unique to them may have resulted in low performance (e.g., small data sets, or data sets that might not be expected to accurately represent the modeled area)? By way of a more specific example to illustrate this point, consider the modeling of Swan Island Lagoon as presented in the report. In this instance, perhaps more weight should be placed on the accuracy of predictions for those species with substantial localized data that would be expected to be most "linked" to the lagoon through diet and home range.

The LWG concern about poor model predictions at smaller spatial scales for fish species with larger home ranges can be addressed by only modeling small home range species during model runs of spatial scales smaller than the entire ISA. It is biologically unrealistic to try and force fish with large home and/or foraging ranges into a spatial area smaller than their home range for modeling purposes. It is more approprite to limit modeling of spatially small areas to fish species such as sculpin with small home ranges.

LWG does not appear to have accepted EPA's suggestions on the first modeling effort in many instances. One example is in the modeling results for black crappie, where EPA suggested that a more zooplankton rich diet be defined for crappie, which have gill rakers specifically designed to capture zooplankton and larval fish from water. One possible cause of the continuing overprediction of contaminant levels in crappie observed in this report is a diet too rich in fish.

Model calibration suggestion: A reading of the dissertations of several of Frank Gobas' graduate students shows that one of the methods they use to improve the agreement between modeled and field collected tissue residues is to change the log Kow value of the chemicals being modeled.

Given the range of measured log Kow values for chemicals in compendia of physical and chemical parameters such as Mackay's 5 volume Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, and the known sensitivity of Gobas type model to changes in log Kow (amply demonstrated in the LWG report), it seems reasonable to adjust the log Kow value in the model so that the measured and model predicted tissue residues are comparable to each other. This is particularly true if the EPA and LWG are satisfied with the values of other model parameters, particularly parameters for which the model is moderately sensitive, such as dietary preferences. A change of 0.3 log units in a log Kow value could give as much as a 2x increase or decrease in predicted tissue residues. As long as the selected log Kow value is reasonable, this is one method to improve the predictive ability of the model.

Develop Understanding of Reasons for Under Prediction of 4,4'-DDE Tissue Concentrations: Additional effort is also required to explain why PCBs can be modeled with some degree of agreement between predicted and measured, but 4,4'-DDE is consistently under-predicted, even using what appears to be a high K<sub>ow</sub>. (The Log K<sub>ow</sub> given in Arnot and Gobas was 5.70, which also results in substantial under-predictions for fish in their application.) The conversion of 4,4'-DDT to 4,4'-DDE may partially account for these inconsistencies. However, there may be additional explanations for instances where source concentrations are not representative (e.g., the actual "active" layer of sediment was not measured, as noted in the report). One approach to determine the source(s) of under-prediction may be to review and compare results for "best" and "worst" predicted species.

<u>Further Evaluate the Role of Surface Water and Relationship Between Surface Water and Sediment</u>: The Food Web Model Report notes the lack of inclusion of a link between the sediment and water concentrations as a weakness in the Arnot and Gobas model. Concentrations in biota are influenced by concentrations in two sources, sediment and water. The report states in Section 6.3.4 that future work will be required to estimate the relative influence of these sources. However, an examination of the coding, as well as the results of the sensitivity analyses should give a fairly clear idea of which species will be estimated by the model to be water- or sediment-source dependent, as well as how that dependence can be altered by changing the diet. It is likely that the sediments in the Willamette River are contributing to the water concentrations and that in some locations or times, the inverse may be true. This issue is important because the fundamental use of the model will be to estimate the changes in biota concentrations resulting from the clean-up of one or more sources.

<u>Refine Sensitivity Analysis with Statistical Approaches</u>: The sensitivity analysis is valuable but could have been done more efficiently with software intended for this purpose such as some type of Monte Carlo software. Although this may not have been possible for TrophicTrace due its "black box" nature (i.e., the model is not an open spreadsheet), focusing on the Arnot & Gobas model, which is an accessible spreadsheet, should allow more efficient sensitivity analysis methods to be used.

<u>Develop Approach to Address Model Limitations Outlined in Section 5.3</u>: Section 5.3 outlines a number of model limitations. However, the report does not include recommendations that address the identified limitations: Limitations and EPA recommendations are outlined below:

- Lack of Phytoplankton and Zooplankton Data: EPA agrees that the lack of phytoplankton and zooplankton data is a significant limitation to the food web model. In fact, EPA identified contaminant concentrations in phytoplankton and zooplankton as a data gap in its December 2, 2005 Round 3 Data Gaps Memo (Data Gaps Memo). It its February 17, 2006 Round 3 Scope of Work (Round 3 SOW), EPA determined that a minimum of four zooplankton tows should be performed to collect zooplankton data for chemical analysis. Contaminant concentrations in phytoplankton may be estimated through the use of appropriate bioconcentration factors.
- <u>Uncertainties Regarding Fish Home Range</u>: EPA agrees that uncertainties regarding fish home range lead to uncertainties in the Food Web Model. It is unclear what steps, if any, are required to address this area of uncertainty.
- <u>Limited Fish Tissue Data</u>: EPA agrees that there is limited fish tissue data with which to run the Food Web Model. In its Data Gaps Memo and Round 3 SOW, EPA has recommended the collection of additional fish tissue composites of representative species (sculpin, largescale sucker, black crappie, smallmouth bass and northern pikeminnow) to support the food web modeling effort and address this limitation.
- Depth to Which Sediment Exposure Occurs: EPA agrees that the definition and characterization of surface sediment concentrations has been shown to be important in adequately modeling contaminant uptake. This active zone is likely to be less than 30 cm. It has been assumed as part of the sediment transport evaluation, that the upper 30 cm of sediment represents, on average, a mixed layer of sediment that is resuspended and redeposited within the Willamette River system in response to episodic events. It is unclear whether further evaluation of the contaminant profile would improve performance of the food web model.
- <u>Dietary Composition</u>: EPA agrees that dietary composition is a key uncertainty in the food web model as well as the dietary approach for evaluating contaminants that are metabolized or otherwise regulated. As stated in EPA's Data Gaps Memo, "Stomach contents analysis will help verify dietary approach parameters, provide information on the type of prey items the fish consumed that are contaminated (important for the food web model), and better represent the specific types of PAHs the fish was exposed to (needed for attributing PAH groupings to sources)." EPA believes that further evaluation of stomach contents will help address this limitation to the food web model.
- <u>Seasonal Variability</u>: EPA agrees that temporal variability in general is a limitation to the food web model. Seasonal variability in surface water data will be addressed through the collection of surface water over two years and a range of flow conditions. In addition, EPA believes that the collection of additional fish tissue data may provide some information regarding fish tissue concentrations over time.

# Improve Model Transparency to Facilitate Agency Review and Public Acceptance:

The key determinant of which platform (i.e., software) to use is transparency, which is defined as the ability for an informed user to follow (if desired) every step of model operation. "Black box" approaches are to be minimized, if not simply avoided. The models should be written in an accessible program like VBA<sup>TM</sup>, with input/output through Excel<sup>TM</sup> spreadsheets, with "elegant" or otherwise "streamlined" coding being discouraged in favor of transparency. The one area where some transparency may be sacrificed is with respect to analysis of uncertainty and sensitivity. For these, use of a EPA Comments on Food Web Modeling Report: Evaluating Trophic Trace and the Arnot and Gobas Models for Application to the Portland Harbor Superfund Site Page 4

Monte Carlo software (e.g., CrystalBall®, @Risk®, etc.) capable of linking to both Excel<sup>TM</sup> spreadsheets and VBA<sup>TM</sup> should be considered. This would considerably simplify the currently cumbersome approach to both of these analyses.

Table 3-1 lists most of the equations used in the Arnot & Gobas model, the model as implemented in the template does not necessarily follow exactly the model described in the literature. For example, the table fails to note that one version of the model uses fugacity concepts to arrive at the final tissue residue estimate and in certain instances (e.g., VLG, VNG, VWG) the table's concise format fails to convey that the results are arrived at as sums of products (e.g., Excel SUMPRODUCT). This indicates that more needs to be done to fulfill the transparency specification, in that each and every equation, parameter, and value used in the actual model must be fully and transparently documented, with more than just a summary table.

Develop and Link Food Web Model to Fate and Transport Model: EPA has previously identified a need for a contaminant fate and transport model that is linked in some way to the food web model. This will allow for predicting future fish tissue concentrations in response to various remediation and source control measures and to estimate how long it will take for fish tissue concentrations to reach protective levels. EPA has developed some guidance on the basic questions that will need to be addressed during development of the Portland Harbor fate and transport and food web models.

### Model Purpose

- 1. Provide managers with information about possible long-term outcomes from various remediation options
- 2. Provide estimates of residue levels in species (e.g., sturgeon, great blue heron) for which empirical data are unlikely to be available.

#### Model Elements

- A simple mass balance fate and transport model linked to food web models will be required. Such a linkage has been accomplished elsewhere. 1
- The fate and transport model can be developed from several variations available in the literature, all of which have proven useful in situations similar to Portland Harbor. <sup>2, 3</sup>
- The food web models should be based on the form initially established by Gobas and subsequently improved by him and others.<sup>4</sup>
- To address the issue of receptor exposures while moving (foraging), divide the harbor into segments within the fate and transport model (see below), develop a

Mackay D, Sang S, Vlahos P, Diamond M, Gobas F and Dolan D. 1994. A rate constant model of chemical dynamics in a lake ecosystem: PCBs in Lake Ontario. Journal of Great Lakes Research 20(4): 625-642.

Davis JA. 2003. The long term fate of PCBs in San Francisco Bay. RMP Technical Report: SFE Contribution 47. San Francisco Estuary Institute, Oakland, CA.

Davis JA. 2004. The long term fate of PCBs in San Francisco Bay. Environmental Toxicology and Chemistry 23(10): 2396-2409.

<sup>&</sup>lt;sup>4</sup> Arnot JA and Gobas FAPC. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. Environmental Toxicology and Chemistry 23(10): 2343-2355.

similar food web model for each segment, and apportion exposure to a mobile receptor as a function of its estimated residence time in each segment.

### Temporal Granularity & Scale

- The models must be dynamic (time-dependent) so that it is possible to track changes over time (in response to possible remedial alternatives) and to determine how long it will take the system to approach steady-state.<sup>5</sup>
- Steady-state only models are not acceptable.
- Both models will need to incorporate seasonally varying data (e.g., river flow rate, water temperature, etc.). A monthly period will provide a reasonable balance between model resolution and the amount of data generated.
- The time increment (dt) must be sufficiently small to capture changes which occur within the course of a time unit (i.e., a month).
- Because of the half-life of some of the contaminants involved, the model should be capable of estimating forward 20-25 years, on a monthly basis.

# Spatial Granularity & Scale

- A multi-segment model is required.<sup>6, 7</sup>
- The model domain should extend from river mile (RM) 11 to RM 2, with a separate compartment for Swan Island Lagoon.
- This domain should be divided into segments, both horizontally and longitudinally, on the basis of appropriate physical parameters.
- Other segmentation patterns (parallel to flow, by habitat, etc.) may be considered after the basic fate and transport model is built.

### Flow Regimes

- USGS data are available from RM 12.8 to provide measures of flow on a daily basis for 30+ years.
- During the summer low flow period, flow reversals and intrusion of Columbia River water can occur. The fate and transport model should be able to accommodate these phenomena at least to the point where there impact on contaminant movement can be assessed.

### Loadings

- The fate and transport model should make provision loads that enter Segment 1 from upstream sources (those above RM 11).
- The fate and transport model should also make provision for including loadings from various sources (e.g., overland, outfalls, groundwater, etc.), even if the quantities of loadings from such sources are currently unknown.

Mackay D. 2001. Multimedia Environmental Models: The Fugacity Approach, Second Edition. 2001. Lewis Publishers, Boca Raton, FL. p.212.

<sup>&</sup>lt;sup>6</sup> See Mackay (2001), p. 210.

Mackay D and Hickie B. 2000. Mass balance model of source apportionment, transport and fate of PAHs in Lac Saint Louis, Quebec. Chemosphere 41: 681-692.

#### Contaminants

- Polychlorinated biphenyls. EPA recognizes the difficulties and uncertainties associated with modeling total PCBs. One suggestion for improving the accuracy of PCB modeling would be to model either homolog groups (e.g. hexachlorobiphenyls), selected individual congeners that are either indicators (among the most abundant individual congeners on a weight percent basis) for specific Aroclor mixtures, which are among the most abundant congeners in higher trophic level fish species (e.g. PCB 138, PCB 153 and PCB 180), 8 or which are among the most toxic PCB congeners (e.g. PCB 126). Depending on the purpose for which a specific model run is being performed (e.g. risk evaluation vs. sediment cleanup goal estimation), LWG may need to model different PCB homologs or congeners at different stages of the RI/FS process. The specific homologs or congeners to be modeled should be cooperatively identified during discussions between EPA and LWG which define specific objectives for a particular set of model runs. Because PCB congener 126 is the most toxic of the PCB congeners and would likely drive the sediment clean-up for PCBs for human health, any food web modeling for risk evaluation purposes should include modeling of PCB 126 as well as other dioxin-like PCBs. This will be necessary to show that development of a remedial goal based upon total PCBs, rather than dioxin -like PCB congeners, would be protective.
- Polycyclic aromatic hydrocarbons. Again, another large group a subset will need to be identified for modeling, as was done for San Francisco Bay. 9, 10 It appears that the metabolism of these contaminants by some aquatic species can be addressed within the type of food web model contemplated here. 11
- Pesticides, represented by 4,4'-DDE, since it is the more toxic, persistent, and bioaccumulative of by-product of 4,4'-DDT. Using Σ4,4'-DDT is not recommended as this can obscure important physicochemical differences among 4,4'-DDT, 4,4'-DDE, and 4,4'-DDD.
- These models are not designed to address metals mechanistically. Metals that are actually expected to biomagnify may be only secondary concern. Modelling methylmercury would require a different, specialized, model, which may not be justified at this time.

#### Food Web Complexity

Greenfield BK and Davis JA. 2004. A simple mass balance model for PAH fate in the San Francisco Estuary. RMP Technical Report, SFEI Contribution 115. San Francisco Estuary Institute, Oakland, CA.

<sup>&</sup>lt;sup>8</sup> See Davis (2003, 2004).

Greenfield BK and Davis JA. 2005. A PAH fate model for San Francisco Bay. Chemosphere 60: 515-530.

Stevenson RW. 2003. Development and application of a model describing the bioaccumulation and metabolism of polycyclic aromatic hydrocarbons in a marine benthic food web. M.S. thesis, School of Resource and Environmental Management, Simon Fraser University, British Columbia, Canada.

Reinfelder JR, Fisher NS, Luoma SN, Nichols JW and Wang WX. 1998. Trace element trophic transfer in aquatic organisms: a critique of the kinetic model approach. Science of the Total Environment 219(2-3): 117-135.

- The Arnot and Gobas formulation of the Gobas food web model is preferred. 13, 14
- An overly detailed food web, with numerous species, is likely to exceed both the availability of site-specific data (i.e., data from 6 fish aren't enough), as well as literature-derived physiological data.
- As the models' primary purpose is to inform remediation decisions and not precisely predict tissue residues, a simplified food web, encompassing representative pelagic and benthic species, should be sufficient at this time.
- A food web model in each segment will address the issue of receptor range and movement.
- Using matrix methods, it is possible to include scavenging and/or cannibalism feeding behaviors in these food webs. 15 However, to minimize model complexity, these feeding relationships should be excluded unless there is a compelling reason to do otherwise.
- Fluctuations in dietary preference can be addressed by normalizing dietary fractions across a "menu" of possible food items. 16

## Data Availability

- The initial goal is a set of integrated working models that capture the principle features of abiotic and biotic fate and transport within the harbor. Achieving working models should not be held hostage to data availability.
- The models should therefore be initially built-out with available site-specific data and appropriate data from the literature. Data gaps should be both identified and filled with information based on best professional judgment. Placeholders should be left for key items (e.g., loadings) which are already known to be important but may not be quantified for some time.
- Sensitivity analysis should be used to narrow our interest in data gaps to those which have the greatest impact on model performance.
- These data gaps can then be addressed in greater detail as the models progress through various editions and refinements.

#### **Specific Comments:**

Page 5, Section 2.1.2, Abiotic Media: It is unclear why total dissolved and particulate concentrations were used in the model (e.g. for surface water) when the individual measurements of both were analyzed for in Portland Harbor sampling (see comment on Section 4.2.1.2 below).

Page 6, Section 2.2.2, Aqueous Uptake: While it is an important exposure route to consider for invertebrates, it is unclear why ventilation of porewater for fish was included in the Arnot and

<sup>&</sup>lt;sup>13</sup> See #4.

Gobas F and Wilcockson J. 2003. San Francisco Bay PCB food-web model. RMP Technical Report, SFE Contribution 90. San Francisco Estuary Institute, Oakland, CA.

<sup>&</sup>lt;sup>15</sup> Sharpe S and Mackay D. A framework for evaluating bioaccumulation in food webs. Environmental Science & Technology 34(12): 2373-2379.

<sup>&</sup>lt;sup>16</sup> USEPA. 2003. Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) Modeling System. Volume I: Modeling System and Science. EPA 530-D-03-001a. Office of Research and Development / Office of Solid Waste, U.S. Environmental Protection Agency, Washington, DC. Section 12, page 12-8.

Gobas model. It is unlikely that any fish would be ventilating porewater at the site, with the *possible* exception of sculpin. For sculpin, the water being ventilated will be a portion of both surface water and transition zone water (as opposed to porewater). More information is needed on the degree to which transition zone water ventilation was considered in the Arnot and Gobas model and for what species.

- Page 8, Section 3.1, Arnot and Gobas (2004): As stated in our general comments on transparency, Table 3-1 does list most of the equations used in the Arnot & Gobas model. However, the model as implemented in the template does not necessarily follow exactly the model described in the literature. This indicates that more needs to be done to fulfill the transparency specification, in that each and every equation, parameter, and value used in the actual model must be fully and transparently documented, with more than just a summary table.
- Page 9, Section 3.3, ECOFATE (Gobas et al. 1998): ECOFATE was offered only as an example of the type of integrated transport & fate / food web model desired for Portland Harbor. EPA acknowledges that ECOFATE is somewhat dated and has limitations. However, its existence (and that of similar models) indicates that such an integrated approach is possible, has been found useful in similar river systems, and could therefore be implemented for Portland Harbor. The absence of loadings data is not a valid reason for rejecting the development and use of such an integrated model, as such information can be estimated with the model and then checked in the field.
- Page 12, Section 4.1.2, Spatial Scales to be Modeled: An average over the entire site (RM 2 RM 11) may easily obscure significant changes occurring over short distances or localized impacts associated with specific sources. Smaller, biologically-defined scales (such as those associated with different fish species) can be accommodated by creating copies of the model at these smaller scales and then pro-rating the results over the scale of each species. Further discussion is required to determine the appropriate scale for the food web model and the factors that should be considered in determining that scale.
- **Page 14, Section 4.2.1, Arnot and Gobas:** It is unclear why the model was altered to accept species-specific porewater ventilation rates for fish expected to be primarily water column feeders, such as black crappie. This scenario may be only appropriate to apply to true benthic fish, such as sculpin. Arnot and Gobas only have crayfish and other invertebrates ventilating porewater, at a generic 5% value. Table 4-3 has the following: 0.2 crayfish, brown bullhead .005, carp .08, black crappie .005, sculpin .02, sucker .08, and juvenile fish 0.01 all based on best professional judgment. In the absence of additional information, Arnot and Gobas recommendations should be followed.
- **Page 14, Section 4.2.1.1, Biological Parameters:** The Arnot & Gobas model is able to model two basic feeding guilds of benthic invertebrates filter feeders & detritivores / scavengers but not necessarily specific species.
- **Page 24, Section 4.4, Model Scenarios:** Because the model is ultimately intended for somewhat generic (FS and planning) purposes, it may be sufficient to use a representative, but simplified, food web throughout the site. It would be more explicit to the reader / reviewer to
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use one food web structure and use uncertainty analysis (e.g. Monte Carlo variables) to represent variability in dietary fractions for each species. Running multiple model runs with differing dietary fractions in order to conduct uncertainty and sensitivity analysis is cumbersome and difficult to review. All scenarios can't be run, leading to uncertainty in terms of the importance of the dietary fraction on the results.

**Page 17, Section 4.2.1.2, Environmental Parameters**: The reference to a MDEQ 2004 document for determining sediment and surface water concentrations from Round 1 and 2 sampling events appears to be in error.

Empirically measured data on environmental parameters should be used over modeled data (e.g. for dissolved oxygen). It is unclear why measurements of TOC, total suspended solids (TSS) and temperature were taken from the ODEQ LASAR database, but not dissolved oxygen data. If available, co-collected TSS and concentration data should be used (isn't TSS data available from the surface water sampling events?).

Page 17, Section 4.2.1.2, Environmental Parameters, Sediment Chemistry: Further clarification regarding the calculation of the area-weighted average should be provided. The methodology to for calculating area-weighted averages is not presented in this report, and cannot be replicated. As stated in the general comment regarding scale, it is unclear whether averaging over large distances is appropriate for this modeling effort. For example, it may not be appropriate to use an average concentration that includes the channel of the river for some species (e.g. smallmouth bass; sculpin) that do not likely inhabit that area.

Page 18, Section 4.2.1.2, Environmental Parameters, Water Chemistry: Only total chemical concentrations were used in the model (sum of concentrations from the XAD filter and water column). In the absence of empirical data on dissolved and particulate concentrations, the model calculates these fractions. However, since empirical data does exist from the XAD analysis, these data should be used in model. The Arnot and Gobas model parameters are: chemical concentration in water (total) and chemical concentration in water (dissolved).

Page 19, Section 4.2.1.2, Environmental Parameters, Water Chemistry: Despite the existence of XAD data in Swan Island Lagoon, surface water data averaged over the entire site was used for the Swan Island model runs (small spatial scale)(see also page 31, Section 5.1.1.2). Site-specific water data from Swan Island should be used in the model runs, especially given the sensitivity to water data in the model. It is not necessary to have a spatially averaged water sample before it is included in the model. It should be noted that EPA has recommended the collection of a surface water transect near the entrance to Swan Island Lagoon in its December 2, 2005 Data Gaps Memo.

**Page 19, Section 4.2.1.2, Environmental Parameters, Water Chemistry:** The text states here that DO, temperature and TSS were calculated from the LASAR database. It should be mentioned here that the DO values were not used in the model (they were calculated using an Arnot and Gobas equation), as indicated on page 17.

- **Page 19, Section 4.2.1.3, Chemical Parameters:** As noted in our general comment regarding under prediction of 4,4'-DDE tissue concentrations, further evaluation of the relationship between 4,4'-DDT and 4,4'-DDE is required. As stated here, a source of 4,4'-4,4'-DDE is 4,4'-4,4'-DDT. One approach for initial modeling purposes is to assume that all 4,4'-DDT is 4,4'-DDE (if 4,4'-DDT is detected in tissue it will be metabolized to 4,4'-DDE), and that 4,4'-DDE is not metabolized (or very little). It may be inappropriate to assume that the conversion of 4,4'-DDT to 4,4'-DDE is balanced out by the metabolism of 4,4'-DDE, since this reaction is very slow.
- Page 20, Section 4.2.2.1, Trophic Trace Biological Parameters: Why are insect larvae, such as chironomids, and crayfish selected for the "water pathway"? These organisms are primarily in direct contact with the sediment. In the case of crayfish, the primary exposure route should be selected, regardless of the existence of a relationship between sediment and tissue (e.g. this could be for other reasons).
- **Page 21, Section 4.2.2.3, Chemical Parameters:** A table that summarizes site specific and literature BSAFs should be included to help understand where literature values used to estimate BSAFs fall in comparison to site specific BSAFs.
- Page 22, Section 4.2, Model Evaluation Methods: Arnot and Gobas (2004) present an evaluation of model performance bias in order to evaluate various modifications to model revisions between the 2004 model and the 1993 model. Model bias is mentioned here, as it is in the Arnot and Gobas publications. However, it is unclear what the basis of the three other model criteria; the species predictive accuracy factor (SPAF), model predictive accuracy factor (MPAF) and the percentage change. Further discussion is required to reach agreement on the criteria used for evaluating the predictive power of the models before the next iteration of the model.
- **Page 25, Section 4.5.1, Sensitivity Analysis:** As stated in our general comment above, the sensitivity analysis would be better served through the use of software intended for this purpose such as some type of Monte Carlo software. Focusing on the Arnot & Gobas model, which is an accessible spreadsheet, should allow these more efficient sensitivity analysis methods to be used.
- Page 27, Section 4.5.2, Uncertainty Analysis: As an uncertainty analysis, this approach seems flawed and not much more than an additional sensitivity analysis. The random selection of a value from within a range of plausible values, where the probability of selection is defined by some distribution, with consideration (when appropriate) for correlation among variables, does not appear to be a factor here. Instead, variables were moved to high or low values as a group, without randomness or regard for potential correlations. Thus, for example, water temperature and TSS are both high simultaneously whereas we know the opposite is true higher summer temperatures coincide with low flows that support lower TSS values. As noted before, focusing on just one model should allow for an actual uncertainty analysis to be performed.
- **Page 28, Section 4.5.2.2, 4,4'-DDE:** Given that 4,4'-DDT is present at the site and in tissue, metabolism of 4,4'-DDT to 4,4'-DDE needs to be represented in the model. The easiest way is to assume measured 4,4'-DDT concentrations are 4,4'-DDE. The text mentions this approach, and then states conversion factors of 20, 50 or 100% 4,4'-DDT were added to the 4,4'-DDE
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- values. However, it is unclear if this analysis was done. The results are not discussed in Section 5.1.3 Section 5.2.1.3.
- **Page 32, Section 5.1.1.4, 4,4'-DDE Swan Island Lagoon:** The Food Web Model Report states that the model is predicting clam issue poorly due to the lack of clam tissue in Swan Island Lagoon. Further iterations of the model using site specific clam tissue collected from Swan Island Lagoon will likely improve model performance.
- Page 25, Section 5.1.2.1, Highly Sensitive Parameters, Percent Moisture and Lipid: Given that percent moisture is a highly sensitive parameter, uncertainty needs to be reduced by using site specific values and ranges for each species.
- Page 52, Section 5.3, 1<sup>st</sup> Paragraph, Surface characterization of Contaminants: As stated in our general comments, the definition and characterization of surface sediment concentrations has been shown to be important in adequately modeling contaminant uptake. EPA agrees that the use of congener data for surface water, and Aroclor data for sediment is a limitation in the modeling effort. This limitation may be addressed through the analysis of archived sediment samples for PCB congeners as part of the Round 2 site characterization efforts.
- **Page 52, Section 5.3, 2<sup>nd</sup> Paragraph, Cannibalism considerations:** Arnot and Gobas describe a method by which scavenging and/or cannibalism can be used in model equations using a matrix solution (Campfens and Mackay, 1997). This method should be incorporated into the modeling effort.
- **Page 52, Section 5.3, Juvenile Compartment:** It is unclear why the juvenile compartment created here included peamouth and black crappie, which juveniles of these species were not collected. Further discussion of how to appropriately address the juvenile compartment is required.
- **Page 57, Section 6.2, Filling Data Gaps:** It is unclear what additional new tools for summarizing sediment chemistry data will be used for future modeling. These methods should be described and discussed with EPA.
- **Page 58, Section 6.2, Time Weighted Averages**: The model should be able to run under different conditions (e.g. different water collection efforts). Time weighted averages should not be used.
- **Page 60, Section 6.3.2, Estimating Time to Recovery:** A time varying model is needed to meet this objective with the appropriate amount of certainty. See general comment.
- **Page 61, Section 6.3.3, Modeling Other Chemicals:** The models can be run with PAHs, with the use of a metabolism factor.
- **Figure 2-1, Dietary and Aquatic Chemical Exposure Pathways:** The following modifications to Figure 2-1 are required:
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- <u>Crayfish</u>: Their diet should include some sediment and detritus. Scavenging should also be included.
- <u>Black Crappie</u>: This species diet should consist mostly of zooplankton (see the Arnot and Gobas supplementary archive where zooplankton are estimated at 75% of total diet). This may be one reason why the model is not predicting tissue concentrations adequately.

# **Table 3-1, Arnot and Gobas Model: Equations:** EPA comments on this table are summarized below:

- <u>Freely Dissolved Chemical Concentration in Porewater</u>: What is the source for this equation? Why is the conc. in sediment multiplied by the density of organic carbon?
- <u>Bioavailable Solute Fraction</u>: Data exists on particulate concentrations in the water.
- <u>Freely Dissolved Chemical Concentration in Surface Water</u>: Dissolved measurements were collected and should be used instead of the equation.
- <u>Freely Dissolved Oxygen Concentration of Water</u>: Empirical measurements exist and should be used in the modeling runs instead of the equation. See also page 19.
- <u>Koc</u>: Why was this equation used to calculate Koc? TrophicTrace uses Log Koc = 0.00028 = 0.983 x Log Kow.

**Table 4-1, Arnot and Gobas, Site Specific Information:** Please see general comment on the use of averages, however, if spatially weighted averages and inverse distance weighting are to be used at any scale, the methodology must be presented and reproducible. Other comments are described below:

- <u>Sediment organic carbon</u>: It is unclear why the values of 1.84 and 2.02 were selected for the ISA and Swan Island Lagoon (e.g. Swan Island value was 2.02 when the mean was 1.86 and the geo mean was 1.42).
- Dissolved / Total Water Concentrations: Use site-specific water concentrations.
- <u>Disequilibrium Factors</u>: Why is a disequilibrium factor of 1 being used for DOC and POC? A disequilibrium factor of 1 would indicate we have evidence that conditions are at equilibrium. Disequilibria between organic carbon and water have been observed for a range or organic chemicals, including PCBs (Arnot and Gobas 2004).

#### **Table 4-3:**

- <u>Diet, all species</u>: See previous comment on diet. We should agree on general representatives for the diet and assume all species can consume from the "representatives" varying amounts. Monte Carlo analysis can be used to interpret the results in terms of uncertainty and sensitivity in diet composition. This will be much easier to interpret. Ranges for parameters such as lipid content, moisture content, and weight should also be used in future model runs.
- Phytoplankton and Zooplankton: Lipid content; non-lipid content, moisture content: In absence of good relevant freshwater values, we should stick with the literature from the Arnot and Gobas model (2004, Supplementary Archive) that references values from Lake Ontario, Lake Erie, and Lake St. Clair. Values listed here for phytoplankton are from the Burrard Inlet in Vancouver BC, a saltwater system, and have low reported lipid and NLOM

- values compared to the Arnot and Gobas values. For zooplankton the referenced values are also for marine organisms from a variety of different sources. A non-lipid organic matter value should be used for zooplankton as well (Arnot and Gobas reports 20%).
- Clam, Crayfish, Insect Larvae, Oligochaete and Fish: Why weren't NLOM values used for these species? Arnot and Gobas demonstrated that "the inclusion of NLOM and water content organism composition fractions as potential storage sites for organic chemicals in fish results in modest increases in the chemical concentrations in fish and subsequent reductions in model error." It would be especially important to use NLOM for organism with low lipid content such as phytoplankton, algae, and invertebrates.